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# Mimetic finite difference methods for diffusion equations on AMR meshes

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# Contents

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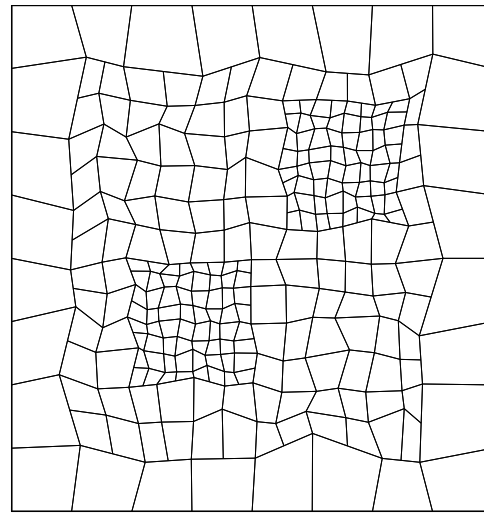
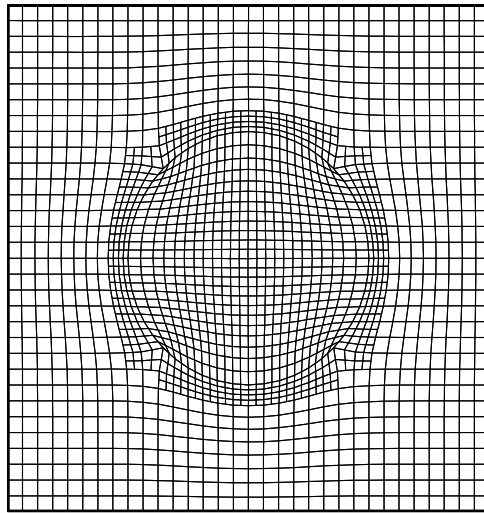
- Objectives
- The support operator method
- Mimetic discretizations on locally refined meshes
- Comparison with other discretization methods
- Recent developments nad future plans
- Conclusions

# Objectives

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What are the perfect discretizations?

- they preserve and mimic mathematical properties of physical systems;
- they are accurate on adaptive smooth and non-smooth grids;

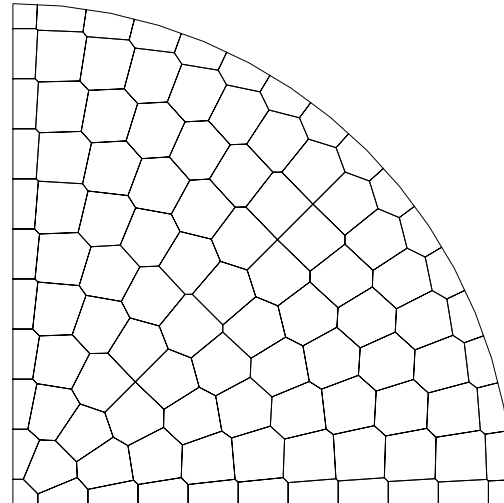
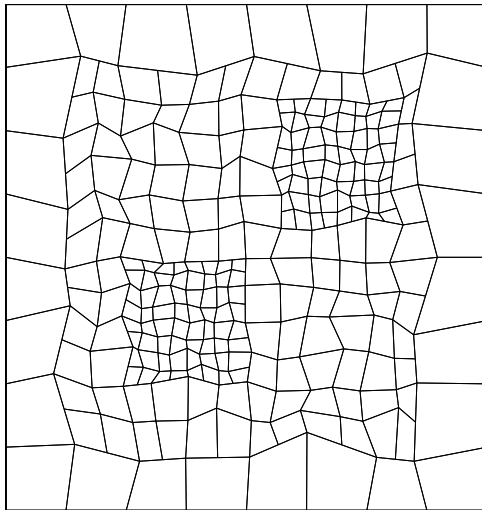


# Objectives

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What are the perfect discretizations?

- they preserve and mimic mathematical properties of physical systems;
- they are accurate on adaptive smooth and non-smooth grids;
- they can be used for a wide family of grids and operators.



# Model diffusion problem

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We consider the elliptic equation

$$-\operatorname{div}(\mathbf{K} \nabla p) = b \quad \text{in} \quad \Omega$$

subject to the homogeneous Dirichlet b.c.

$$p = 0 \quad \text{on} \quad \partial\Omega.$$

The problem can be reformulated as a system of first order equations:

$$\begin{aligned} \operatorname{div} \mathbf{f} &= b, \\ \mathbf{f} &= -\mathbf{K} \nabla p. \end{aligned}$$

For simplicity we assume that  $\mathbf{K} = \mathbf{I}$ .

# Support operator method (1/2)

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Consider the mathematical identity:

$$\int_{\Omega} \operatorname{grad} p \, \mathbf{f} \, dx = - \int_{\Omega} \operatorname{div} \mathbf{f} \, p \, dx \quad \forall \mathbf{f} \in H_{div}(\Omega), p \in H_0^1(\Omega).$$

Support-operators (SO) methodology (for div & grad):

1. define degrees of freedom for variables  $p$  and  $\mathbf{f}$ ;
2. equip the discrete spaces for  $p$  and  $\mathbf{f}$  with scalar products  $[\cdot, \cdot]_Q$  and  $[\cdot, \cdot]_X$ , respectively;
3. choose a discrete approximation to the divergence operator, the *prime* operator **DIV**:  $X_d \rightarrow Q_d$ ;
4. derive the discrete approximation of the gradient operator, the *derived* operator **GRAD**:  $Q_d \rightarrow X_d$ , from the discrete Green formula:

$$[f^d, \mathbf{GRAD} p^d]_X = -[\mathbf{DIV} f^d, p^d]_Q \quad \forall p^d \in Q_d, f^d \in X_d.$$

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# Support operator method (2/2)

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Applications of the SO methodology include:

- Electromagnetics: discrete operators **DIV**, **GRAD**, **CURL** and **CURL** mimic:

$$\text{div curl} = 0, \quad \text{curl grad} = 0$$

$$\int_{\Omega} \text{curl} \mathbf{E} \cdot \mathbf{H} \, dx = \int_{\Omega} \text{curl} \mathbf{H} \cdot \mathbf{E} \, dx + \oint_{\partial\Omega} (\mathbf{E} \times \mathbf{H}) \cdot \mathbf{n} \, ds$$

- CFD: discrete operators **DIV** and **GRAD** mimic:

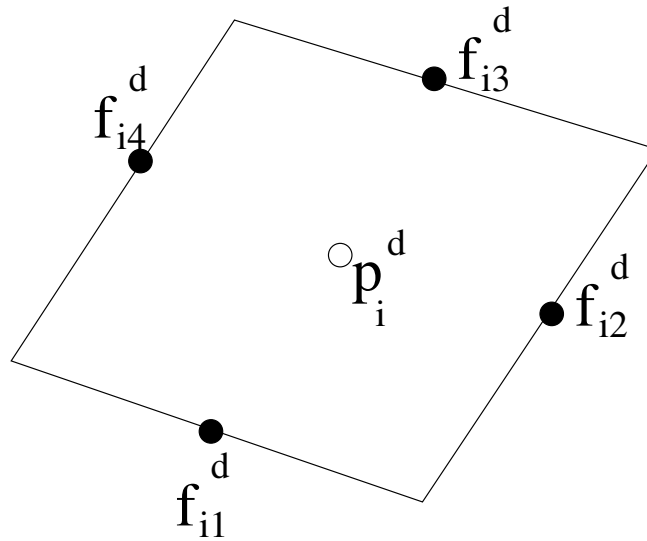
$$\int_{\Omega} \text{grad} \mathbf{u} : \mathbf{T} \, dx = - \int_{\Omega} \text{div} \mathbf{T} \cdot \mathbf{u} \, dx + \oint_{\partial\Omega} \mathbf{u} \cdot (\mathbf{T} \cdot \mathbf{n}) \, ds$$

- Gas dynamics, poroelasticity, magnetic diffusion, radiation diffusion, etc...

<http://www.sci.sdsu.edu/compscims/MIMETIC/index.htm>

# Mimetic discretizations (1/10)

Step 1 (degrees of freedom for  $p$  and  $\mathbf{f}$ ).



- $p_i^d$  is defined at a center of cell  $e_i$ .
- $f_{i1}^d, \dots, f_{i4}^d$  are defined at mid-points of cell edges. They approximate the normal components of  $\mathbf{f}$ , e.g.

$$f_{i1}^d \approx \mathbf{f} \cdot \mathbf{n}_{i1}.$$

# Mimetic discretizations (2/10)

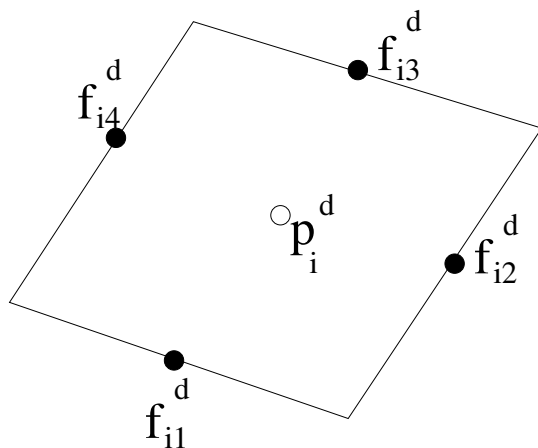
Step 2 (scalar products for  $p^d$  and  $f^d$ ).

- Let  $Q_d$  be a vector space of discrete intensities with the scalar product

$$[p^d, q^d]_Q = \sum_{i=1}^N |e_i| p_i^d q_i^d \approx \int_{\Omega} p(x) q(x) dx.$$

- Let  $X_d$  be a vector space of discrete fluxes with a scalar product

$$[f^d, g^d]_X \approx \int_{\Omega} \mathbf{f}(x) \cdot \mathbf{g}(x) dx.$$



The vectors can be recovered uniquely at four vertices of quadrilateral  $e_i$ . Let

$$[f_i^d, g_i^d]_{X_{e_i}} = \frac{1}{2} \sum_{j=1}^4 |T_{ij}| \mathbf{f}_{ij}^d \cdot \mathbf{g}_{ij}^d$$

$$\text{Then } [f^d, g^d]_X = \sum_{i=1}^N [f_i^d, g_i^d]_{X_{e_i}}.$$

# Mimetic discretizations (2/10)

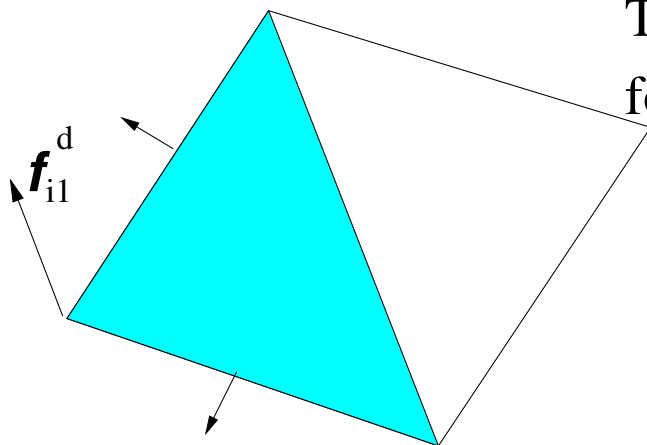
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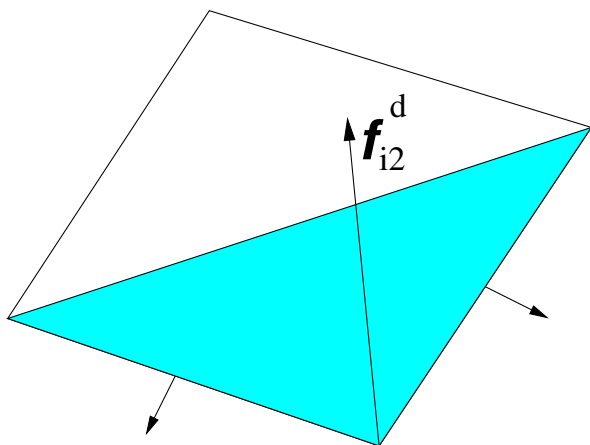
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Step 2 (scalar products for  $p^d$  and  $f^d$ ).

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- Let  $X_d$  be a vector space of discrete fluxes with a scalar product
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$$[f_i^d, g_i^d]_{X_{e_i}} = \frac{1}{2} \sum_{j=1}^4 |T_{ij}| \mathbf{f}_{ij}^d \cdot \mathbf{g}_{ij}^d$$

$$\text{Then } [f^d, g^d]_X = \sum_{i=1}^N [f_i^d, g_i^d]_{X_{e_i}}.$$

# Mimetic discretizations (2/10)

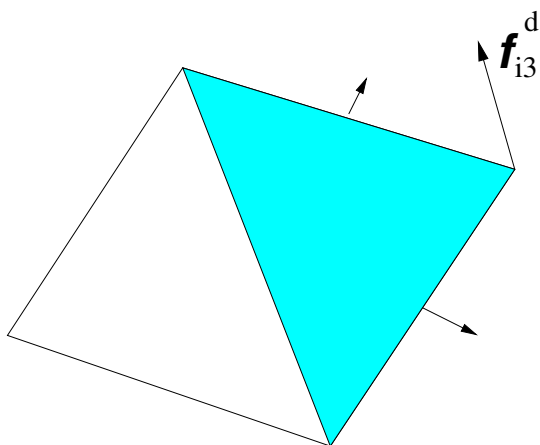
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- Let  $X_d$  be a vector space of discrete fluxes with a scalar product

$$[f^d, g^d]_X \approx \int_{\Omega} \mathbf{f}(x) \cdot \mathbf{g}(x) dx.$$



The vectors can be recovered uniquely at four vertices of quadrilateral  $e_i$ . Let

$$[f_i^d, g_i^d]_{X_{e_i}} = \frac{1}{2} \sum_{j=1}^4 |T_{ij}| \mathbf{f}_{ij}^d \cdot \mathbf{g}_{ij}^d$$

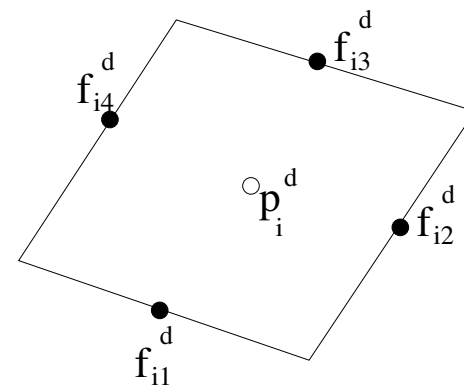
$$\text{Then } [f^d, g^d]_X = \sum_{i=1}^N [f_i^d, g_i^d]_{X_{e_i}}.$$

# Mimetic discretizations (3/10)

Steps 3 & 4 (prime and derived operators).

The prime operator **DIV** follows from the Gauss theorem:

$$\operatorname{div} \mathbf{f} = \lim_{|e| \rightarrow 0} \frac{1}{|e|} \oint_{\partial e} \mathbf{f} \cdot \mathbf{n} \, dl.$$



Center-point quadrature gives

$$(\mathbf{DIV} f^d)_i = \frac{1}{|e_i|} (f_{i1}^d |l_1| + f_{i2}^d |l_2| + f_{i3}^d |l_3| + f_{i4}^d |l_4|)$$

The derived operator **GRAD** is implicitly given by

$$[f^d, \mathbf{GRAD} p^d]_X = -[\mathbf{DIV} f^d, p^d]_Q \quad \forall p^d \in Q_d, f^d \in X_d.$$

# Mimetic discretizations (4/10)

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Short summary.

The stationary diffusion problem

$$\begin{aligned} -\operatorname{div} \mathbf{K} \nabla p &= b & \text{in } \Omega \\ p &= 0 & \text{on } \partial\Omega \end{aligned}$$

is rewritten as the 1st order system

$$\mathbf{f} = -\mathbf{K} \nabla p, \quad \operatorname{div} \mathbf{f} = b$$

and discretized as follows:

$$\mathbf{f}^d = -\text{GRAD } p^d, \quad \text{DIV } \mathbf{f}^d = b^d.$$

# Mimetic discretizations (5/10)

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By the definition,

$$[f^d, \text{GRAD } p^d]_X = -[\text{DIV } f^d, p^d]_Q.$$

Let  $\langle \cdot, \cdot \rangle$  be the usual vector dot product. Then

$$[p^d, q^d]_Q = \langle \mathcal{D}p^d, q^d \rangle, \quad [f^d, g^d]_X = \langle \mathcal{M}f^d, g^d \rangle.$$

Combining the last two formulas, we get

$$\begin{aligned} [f^d, \text{GRAD } p^d]_X &= \langle \mathcal{M}f^d, \text{GRAD } p^d \rangle \\ &= -[\text{DIV } f^d, p^d]_Q = -\langle f^d, \text{DIV}^t \mathcal{D}p^d \rangle. \end{aligned}$$

Therefore,

$$\text{GRAD} = -\mathcal{M}^{-1} \text{DIV}^t \mathcal{D}.$$

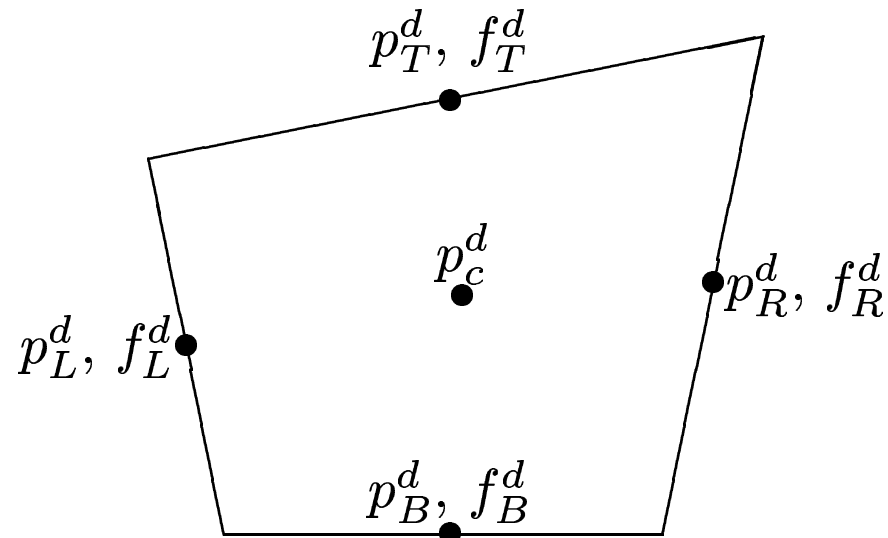
# Mimetic discretizations (6/10)

A local SO method mimics the mathematical identity

$$\int_e \mathbf{f} \cdot \text{grad} p \, dx + \int_e \text{div} \mathbf{f} p \, dx = \int_{\partial e} p \mathbf{f} \cdot \mathbf{n} \, dl.$$

Step 1 (degrees of freedom):

- $p^d$ : at cell centers and edge centers
- $f^d$ : normal components at edge centers



# Mimetic discretizations (7/10)

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Steps 2 & 3 (discrete identity and prime operator).

The prime operator **DIV** is derived from the Gauss theorem:

$$\mathbf{DIV} f^d = \frac{1}{|e|} (f_R^d |l_R| + f_T^d |l_T| + f_L^d |l_L| + f_B^d |l_B|)$$

Derivation of the discrete identity:

- $\int_e \mathbf{f} \cdot \text{grad} p \, dx \approx [f^d, \mathbf{GRAD} p^d]_{X_e}$
- $\int_e \text{div} \mathbf{f} p \, dx \approx (\mathbf{DIV} f^d) p_c^d |e|$
- $\int_{\partial e} p \mathbf{f} \cdot \mathbf{n} \, dl \approx p_R^d f_R^d |l_R| + p_T^d f_T^d |l_T| + p_L^d f_L^d |l_L| + p_B^d f_B^d |l_B|$

# Mimetic discretizations (8/10)

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Step 4 (derived operator).

Replacing integrals in the Green formula by their approximations, we get

$$\text{GRAD } p^d = \mathcal{M}_e^{-1} \begin{pmatrix} |l_R|(p_R^d - p_c^d) \\ |l_T|(p_T^d - p_c^d) \\ |l_L|(p_L^d - p_c^d) \\ |l_B|(p_B^d - p_c^d) \end{pmatrix}$$

where

$$\langle \mathcal{M}_e f^d, g^d \rangle = [f^d, g^d]_{X_e}$$

and  $f^d = (f_R^d, f_T^d, f_L^d, f_B^d)^t$ . The local discretization reads

$$\text{DIV } f^d = b^d,$$

$$f^d = -\text{GRAD } p^d.$$

# Mimetic discretizations (9/10)

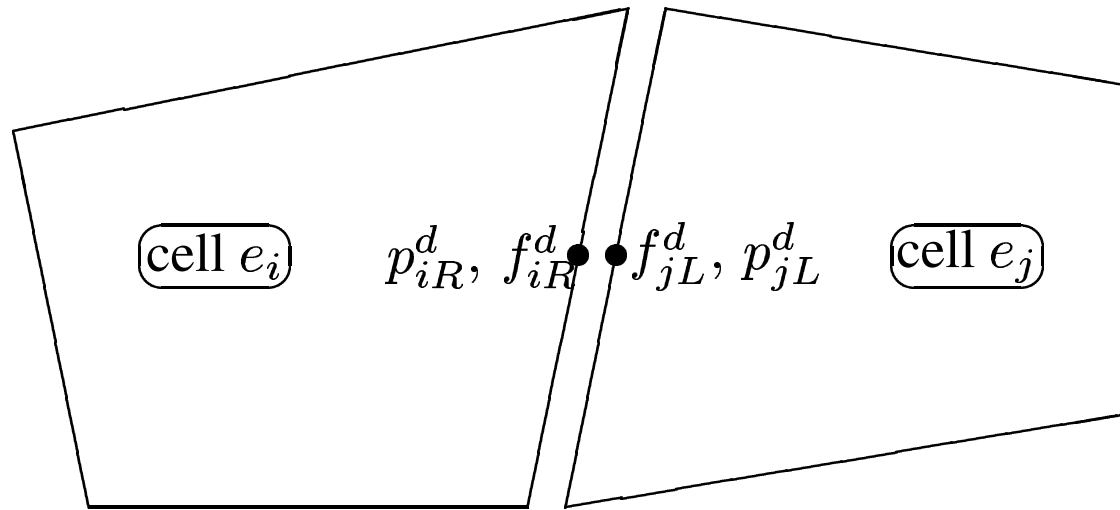
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## Short summary.

- matrix  $M_e^{-1} \in \mathbb{R}^{4 \times 4}$ ;
- discrete divergence and gradient operators mimic essential properties of the continuous operators (local mass conservation, Green formula);
- discretization and continuity conditions are separated;
- we do not assume anything about a grid structure.

# Mimetic discretizations (10/10)

$$\int_{\partial e} p \mathbf{f} \cdot \mathbf{n} \, dl \approx p_R^d f_R^d |l_R| + p_T^d f_T^d |l_T| + p_L^d f_L^d |l_L| + p_B^d f_B^d |l_B|.$$



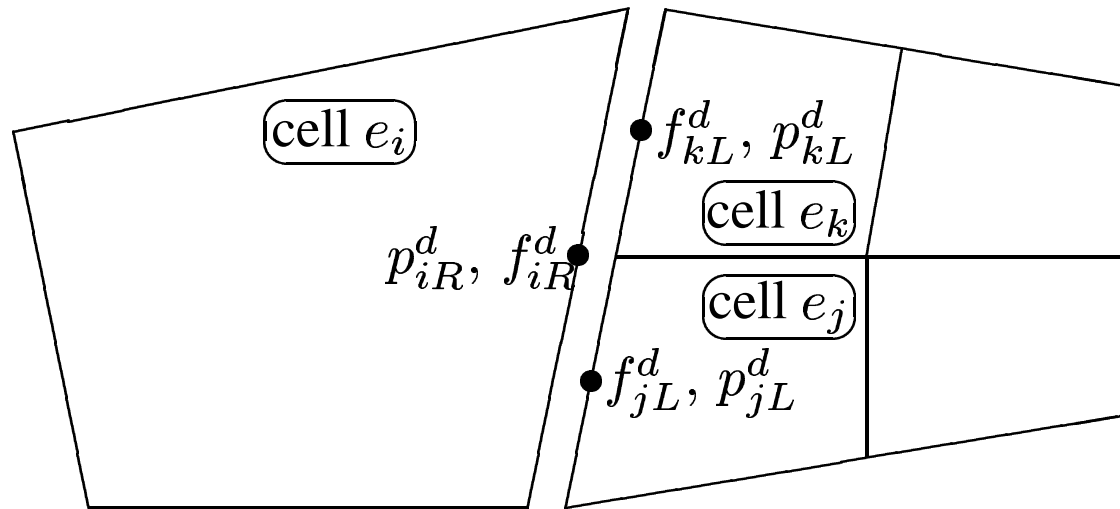
The global discretization is achieved by imposing the continuity of fluxes

$$f_{iR}^d = -f_{jL}^d$$

and interface intensities

$$p_{iR}^d = p_{jL}^d.$$

# Locally refined meshes (1/6)



The global discretization is achieved by imposing the continuity of fluxes

$$f_{iR}^d = -f_{jL}^d = -f_{kL}^d$$

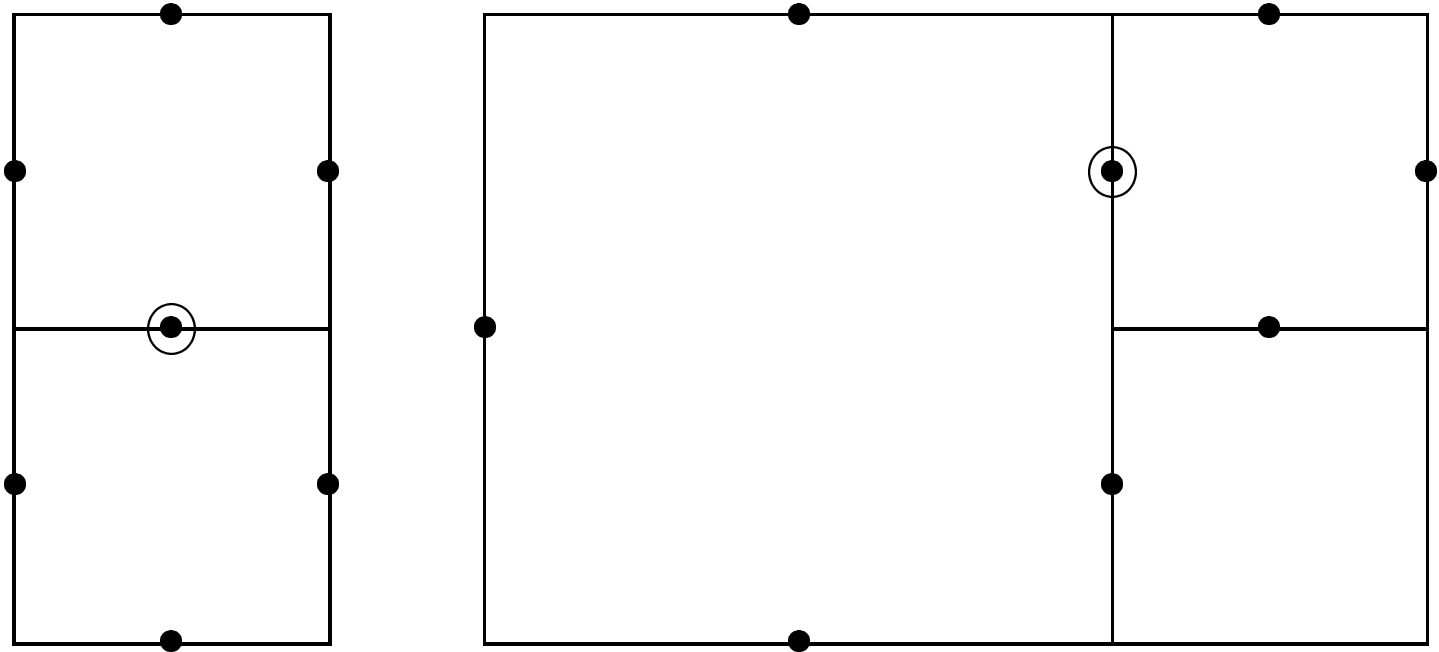
and interface intensities

$$|l_{iR}| p_{iR}^d = |l_{jL}| p_{jL}^d + |l_{kL}| p_{kL}^d.$$

# Locally refined meshes (2/6)

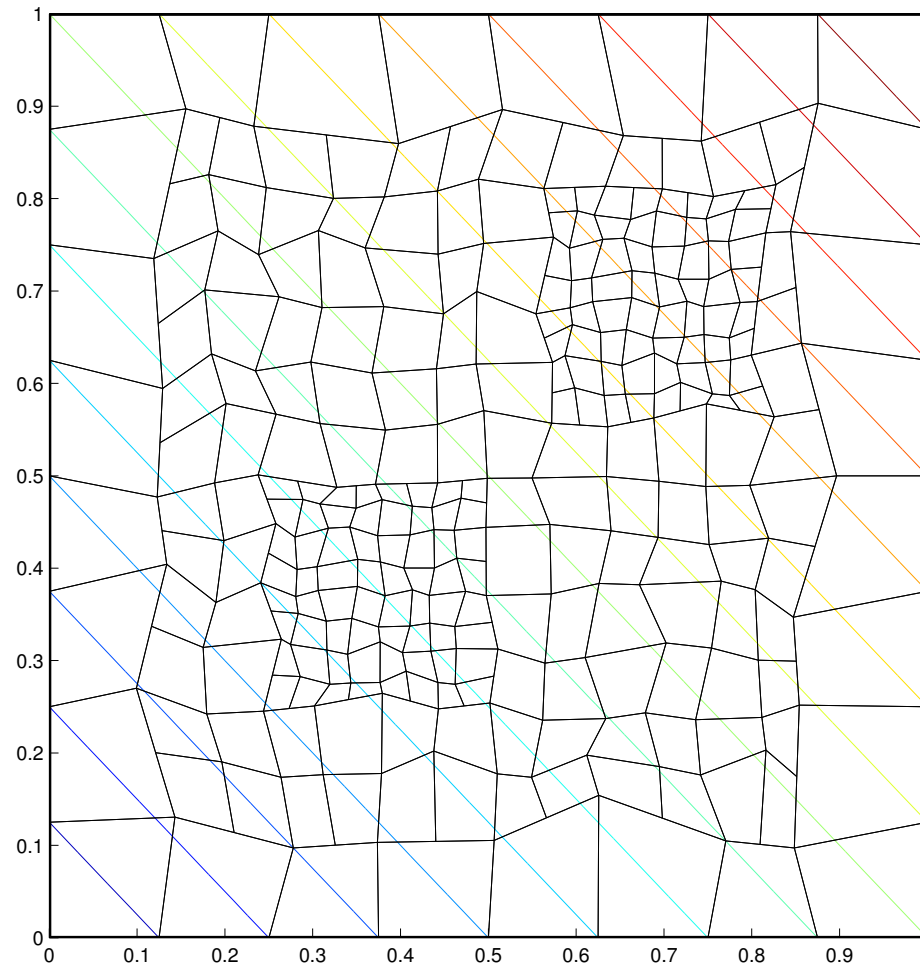
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Stencils of a stiffness matrix for interface intencities.

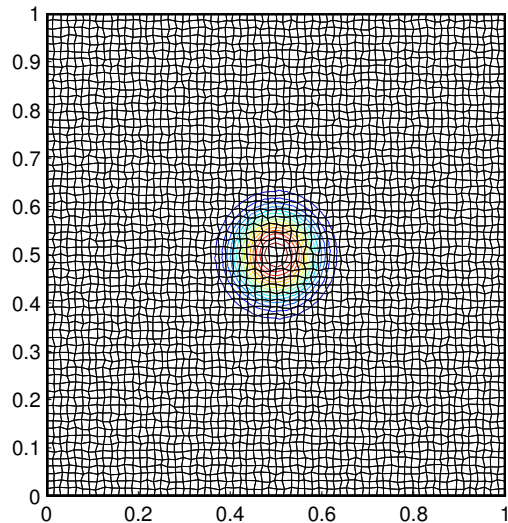
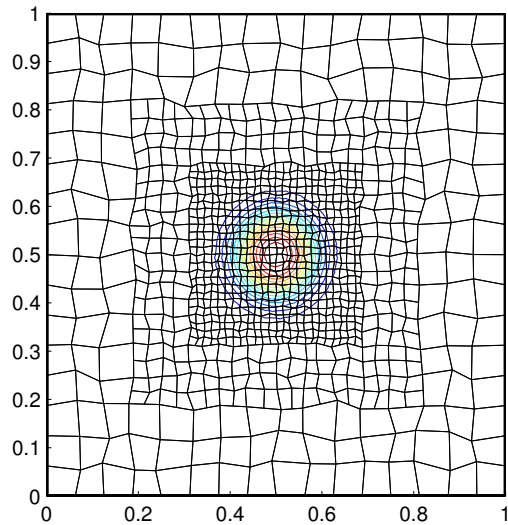


# Locally refined meshes (3/6)

The derived mimetic discretizations are exact for linear solutions.



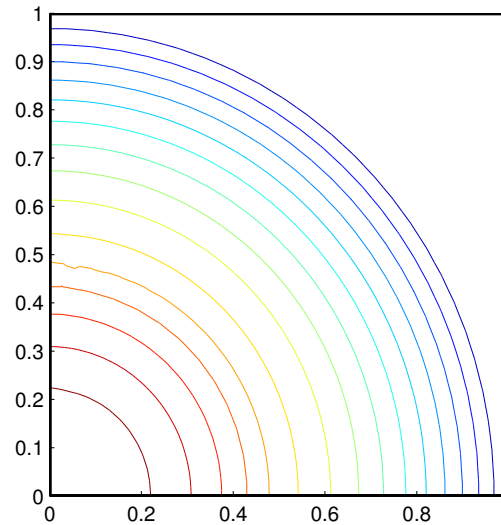
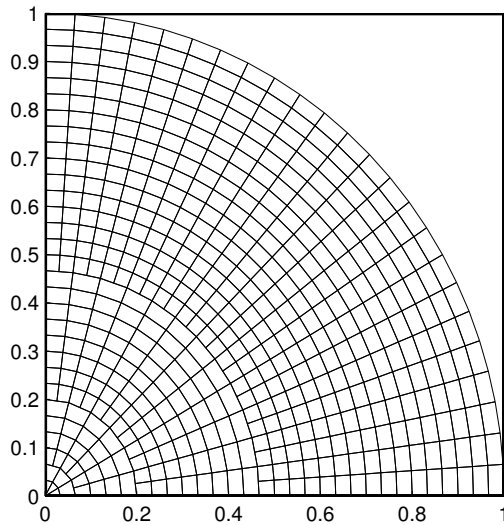
# Locally refined meshes (4/6)



$l$	$N$	$\varepsilon_p$	$\varepsilon_f$	#itr	CPU,s
AMR grids					
0	256	7.00e-2	8.18e-2	12	0.05
1	556	1.64e-2	3.42e-2	15	0.14
2	988	3.74e-3	1.74e-2	16	0.28
3	3952	9.96e-4	7.57e-3	16	1.33
4	<u>15808</u>	2.40e-4	3.79e-3	17	6.21
Uniform grids					
0	256	7.00e-2	8.18e-2	12	0.05
1	1024	1.79e-2	3.40e-2	13	0.27
2	4096	3.91e-3	1.62e-2	14	1.25
3	16384	9.44e-4	7.30e-3	15	5.58
4	<u>65536</u>	2.32e-4	3.76e-3	17	25.3

$$p(x, y) = 1 - \tanh \left( \frac{(x - 0.5)^2 + (y - 0.5)^2}{0.01} \right).$$

# Locally refined meshes (5/6)



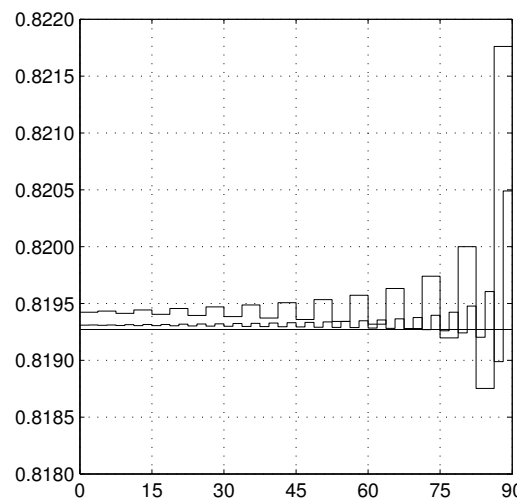
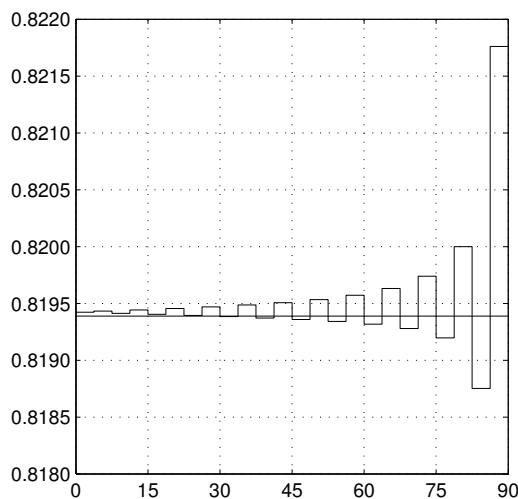
Spherically symmetric problem in  $r - z$  coordinates with the exact solution:

$$p(R) = \frac{553}{640} - \frac{R^2}{6} - \frac{R^4}{20}$$

when  $R < 0.5$  and

$$p(R) = \frac{101}{120} - \frac{R^2}{12} - \frac{R^4}{40}$$

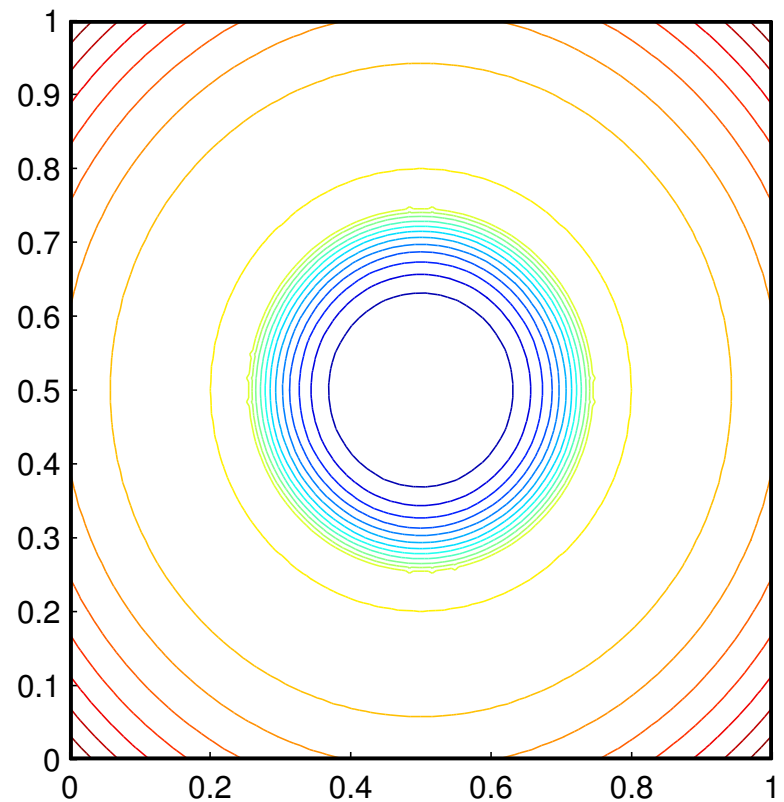
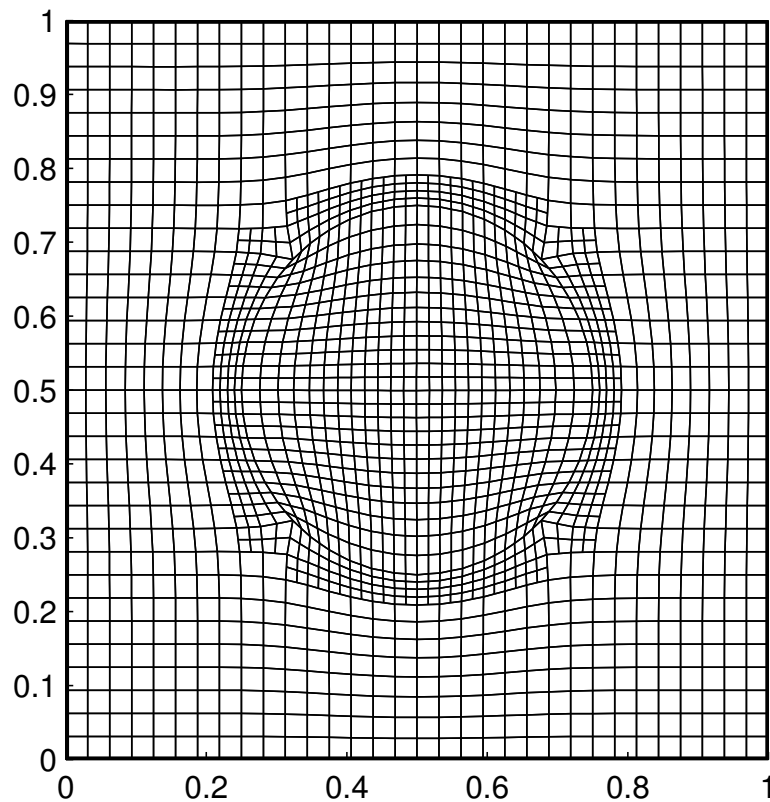
when  $0.5 < R < 1$ .



# Locally refined meshes (6/6)

Let us consider the diffusion problem with strong material discontinuity

$$[K] = 100 \quad \text{at} \quad \sqrt{(x - 0.5)^2 + (y - 0.5)^2} = 0.25.$$



# SO and mixed FE methods (1/3)

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The system of mimetic finite difference equations

$$f^d = -\text{GRAD } p^d, \quad \text{DIV } f^d = b^d$$

can be rewritten as

$$\begin{aligned} [f^d, g^d]_X + [\text{GRAD } p^d, g^d]_X &= 0, \\ [\text{DIV } f^d, q^d]_Q &= [b^d, q^d]_Q. \end{aligned}$$

Recall that by the definition,

$$[f^d, \text{GRAD } p^d]_X = -[\text{DIV } f^d, p^d]_Q.$$

# SO and mixed FE methods (2/3)

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Thus, the mimetic discretizations are equivalent to

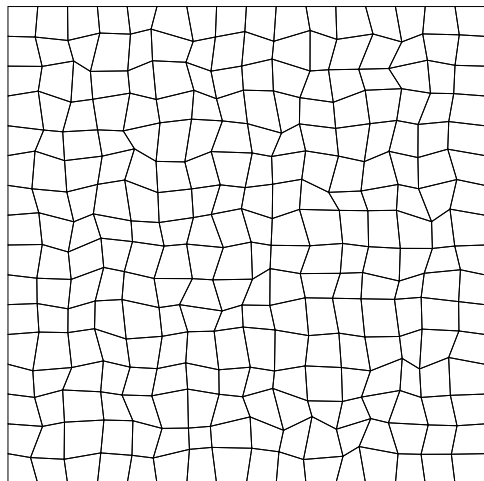
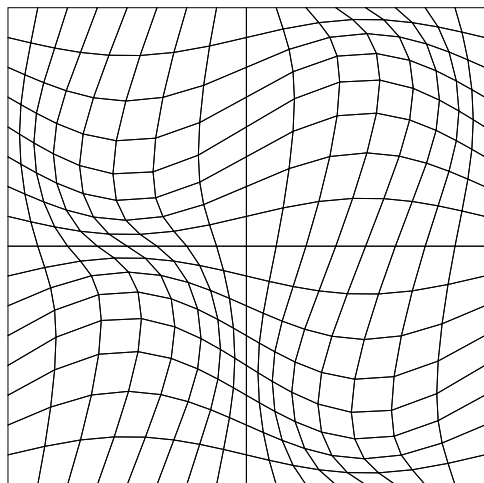
$$\begin{aligned} [f^d, g^d]_X - [\text{DIV } f^d, p^d]_Q &= 0, \\ -[\text{DIV } f^d, q^d]_Q &= -[b^d, q^d]_Q, \quad \forall p^d \in Q_d, g^d \in X_d. \end{aligned}$$

On the other hand, the MFE method with the *Raviart-Thomas* elements gives

$$\begin{aligned} (f^h, g^h) - (\text{div } f^h, p^h) &= 0, \\ -(\text{div } f^h, q^h) &= -(b, q^h) \quad \forall q^h \in Q_h, g^h \in X_h. \end{aligned}$$

	$p^d$ :	at cell centers	one per cell
Degrees of freedom:	$f^d$ :	normal components at edge centers	normal components, one per edge

# SO and mixed FE methods (3/3)

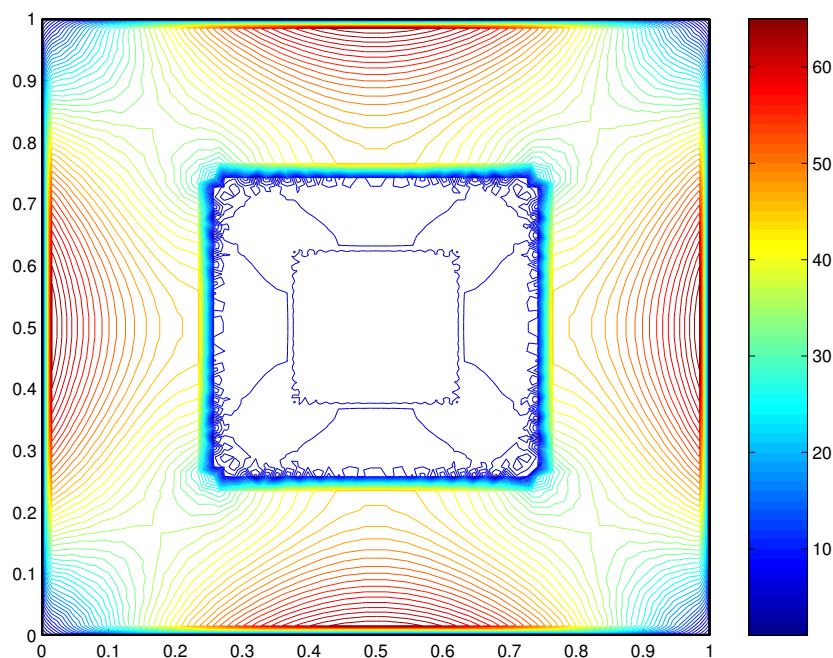
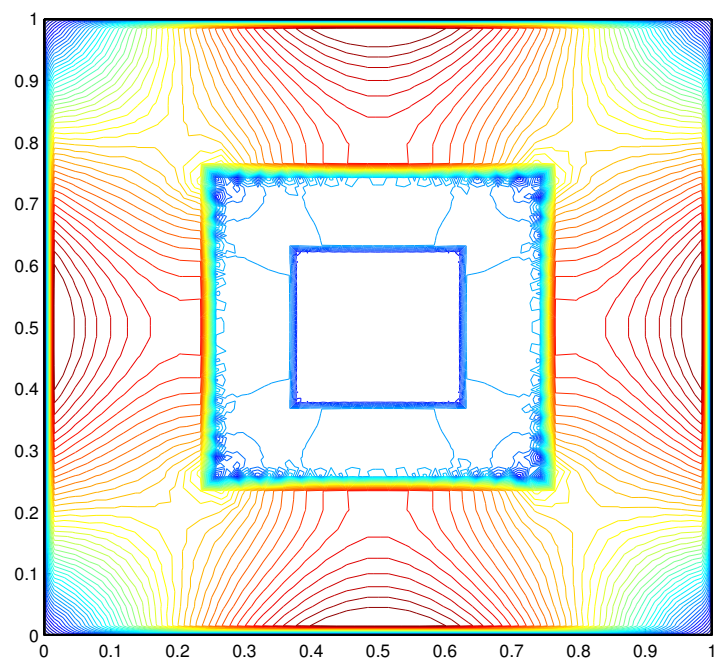


$h^{-1}$	modified RT FE		SO FD	
	$\varepsilon_p$	$\varepsilon_f$	$\varepsilon_p$	$\varepsilon_f$
16	1.58e-3	2.34e-2	1.61e-3	2.35e-2
32	7.95e-4	1.22e-2	7.99e-4	1.22e-2
64	3.98e-4	6.29e-3	3.99e-4	6.29e-3
128	1.99e-4	3.22e-3	1.99e-4	3.22e-3
256	9.97e-5	1.64e-3	9.97e-5	1.64e-3
512	4.98e-5	8.32e-4	4.98e-5	8.32e-4
	$\varepsilon_p$	$\varepsilon_f$	$\varepsilon_p$	$\varepsilon_f$
16	1.42e-3	2.24e-2	1.43e-3	2.25e-2
32	7.15e-4	1.17e-2	7.18e-4	1.17e-2
64	3.59e-4	5.96e-3	3.59e-4	5.98e-3
128	1.80e-4	3.06e-3	1.80e-4	3.07e-3
256	9.00e-5	1.56e-3	9.00e-5	1.56e-3
512	4.50e-5	7.93e-4	4.50e-5	7.93e-4

# SO and FD methods (1/1)

In collaboration with M.Pernice (CCS-3), the SO method was compared with the FD method by R.Ewing, R.Lazarov, and P.Vassilevki (1991):

- the FD method works on rectangular locally refined grids;
- in the case of smooth solutions, the FD method results in larger error (left picture) on irregular grid interfaces:



# SO and CV methods (1/1)

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The control-volume mixed FE method by T.Russell (2001):

- the method does not preserve the uniform flow on irregular grids;
- the principle difficulty is the scalar product in a space of fluxes.

The control-volume method on general polygonal meshes by T.Palmer (2001):

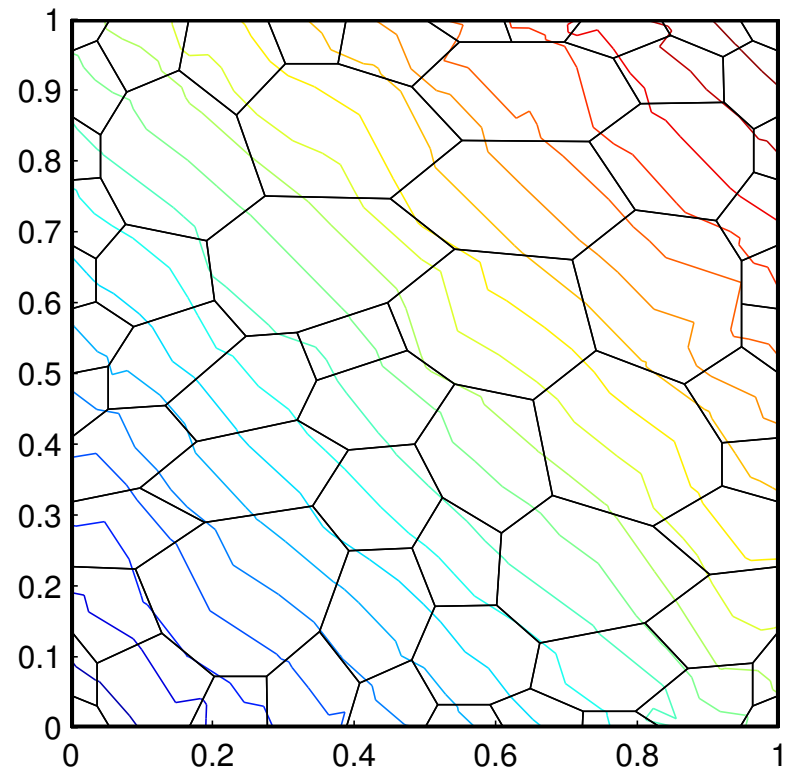
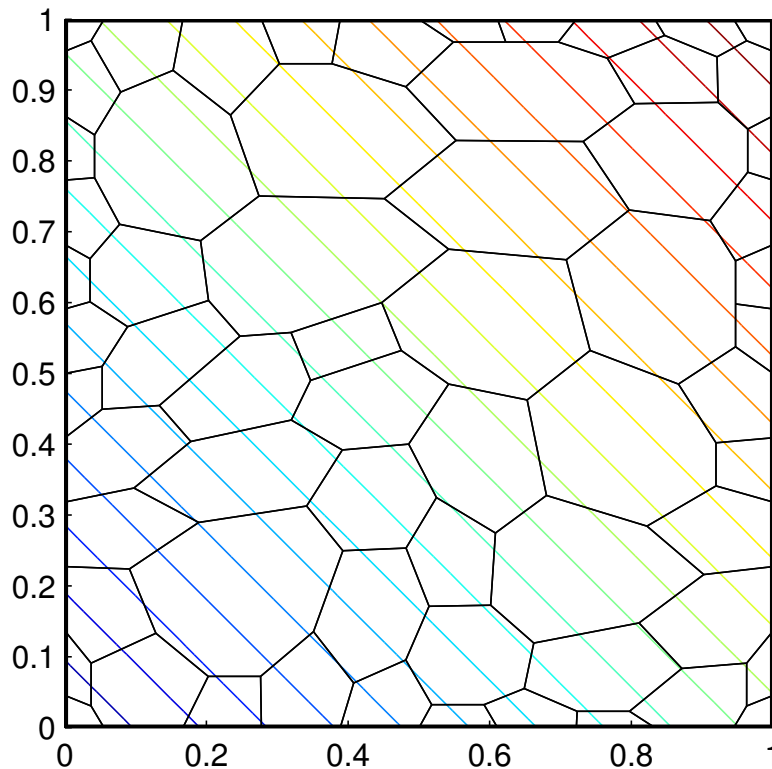
- the method is exact for linear solutions;
- the method results in non-symmetric matrices.

The SO method on general polygonal meshes (2003):

- the method is exact for linear solutions;
- the method results in symmetric positive definite matrices.

# Recent developments (1/3)

Exact solution is  $p(x, y) = x + y$ . A new scalar product in the space of fluxes results in mimetic discretizations which are exact for linear solutions.

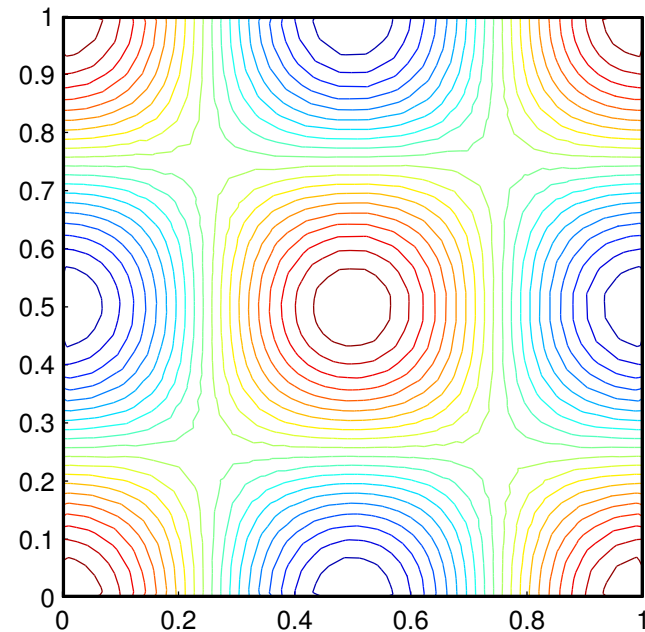
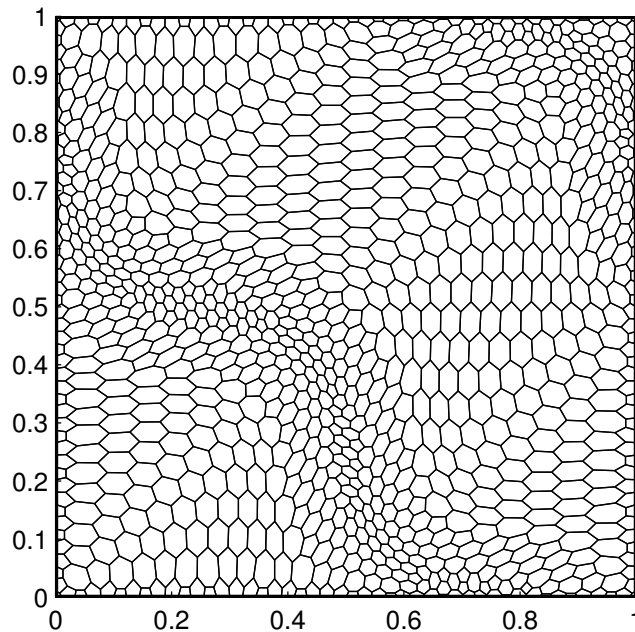


The polygonal grids were generated by Raphael Loubere (T-7).

# Recent developments (2/3)

Convergence test for exact solution  $p(x, y) = \sin(2\pi x) \sin(2\pi y)$ .

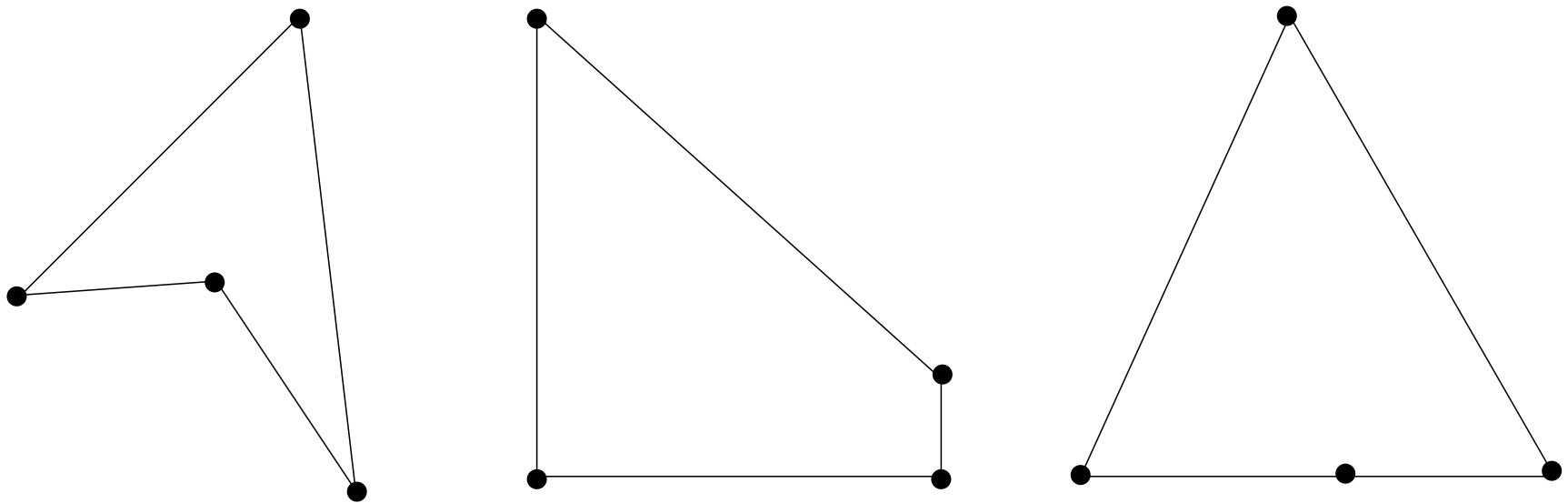
$m$	New scalar product		Old scalar product	
	$\varepsilon_p$	$\varepsilon_f$	$\varepsilon_p$	$\varepsilon_f$
166	1.07e-1	3.68e-1	1.81e-1	4.57e-1
598	2.60e-2	1.64e-1	3.39e-2	2.52e-1
2230	5.11e-3	8.28e-2	6.64e-3	1.72e-1
8566	1.05e-3	4.29e-2	1.51e-3	1.20e-1



# Recent developments (3/3)

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Examples of bad-shaped elements which are common for locally refined and non-matching meshes:



We believe that the new methodology can be extended to all the above elements.

# Conclusion

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- the convergence of mimetic discretizations for the linear diffusion equation is optimal on locally refined meshes in both Cartesian and  $r - z$  geometries (2nd order on smooth meshes but only 1st order for fluxes on random grids);
- the mimetic discretizations are comparable with mixed FE discretizations but more preferable than the discretizations based on CV or FD methods;
- a reduced system for interface intensities has SPD coefficient matrix and can be efficiently solved with a PCG method;
- the preliminary numerical experiments on general polygonal meshes show the optimal convergence rate for mimetic discretizations (2nd order for intensities and 1st order for fluxes).